

Butyl ether  
142-96-1 | DTXSID1022007

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

## Model Results

**Predicted value:**  $2.21 \times 10^{-11}$  cm<sup>3</sup>/molecule\*sec

**Global applicability domain:** Inside

**Local applicability domain index:**  $7.53 \times 10^{-1}$

**Confidence level:**  $8.63 \times 10^{-1}$

## Nearest Neighbors from the Training Set

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Butyl ether

**Measured:**  $2.88 \times 10^{-11}$

**Predicted:**  $2.21 \times 10^{-11}$

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Propane, 1,1'-oxybis[2-methyl-

**Measured:**  $2.60 \times 10^{-11}$

**Predicted:**  $2.13 \times 10^{-11}$

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1-Heptanol

**Measured:**  $1.37 \times 10^{-11}$

**Predicted:**  $1.45 \times 10^{-11}$

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1-Octanol

**Measured:**  $1.44 \times 10^{-11}$

**Predicted:**  $1.66 \times 10^{-11}$